



U.S. DEPARTMENT OF
ENERGY

Nuclear Energy

Advanced Safety Modeling

Coupling of High Fidelity and Integral Analysis Methods

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AFCI NEAMS Meeting

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Highlights

■ Objective

- Provide high-fidelity reactor and plant safety analysis models for integration into the advanced simulation code framework.
- Utilize existing safety simulation tools coupled with emerging high-fidelity modeling capabilities to quantify critical safety-related phenomenon in advanced reactor designs.

■ FY09 Milestones

- 7/31 (M2): Coupling of High Fidelity and Integral Analysis Methods (ANL-AFCI-269).
- 9/30 (M3): Prototypic Analyses Demonstrating Coupled Safety Modeling (ANL-AFCI-279).

■ FY09 Funding

- Initial funding level: \$450k.
- Funding increase: \$100k.

9/30 (M3): Global Sensitivity Metrics and Efficient Methods for Their Evaluation (ANL-AFCI-293).

**Uncertainty
Quantification for
Nuclear Engineering
Applications**

Advanced Fuel Cycle Initiative

**Initial Coupling of High
Fidelity and Integral
Analysis Methods**

Advanced Fuel Cycle Initiative

Prepared for
U.S. Department of Energy
and Simulation Campaign
Initiative, O. Roderick
Argonne National Laboratory
September 23, 2009
ANL-AFCI-269

**Demonstration of
Coupled Safety Modeling
Using High Fidelity
Methods**

Advanced Fuel Cycle Initiative

Prepared for
Department of Energy
and Simulation Campaign
Initiative, H. Fanning and T. Sofu
Argonne National Laboratory
July 31, 2009
ANL-AFCI-279

Prepared for
U.S. Department of Energy
Modeling and Simulation Campaign
T. H. Fanning, T. Sofu, and F. E. Dunn
Argonne National Laboratory
September 25, 2009
ANL-AFCI-279

This document contains preliminary information and must be reviewed by the originating facility before public release.



Global Sensitivity Evaluations

- **A polynomial regression technique has been developed that makes use of derivative information to efficiently evaluate global sensitivity metrics.**
 - Standard methods use large-scale sampling, or tangent linear models with derivatives computed based on finite differences.
 - Requires many more code executions.
- **Challenge: Automatically evaluate derivatives based on existing, complex computer codes with minimal code modifications.**
- **Automatic Differentiation (AD)**
 - Code in Fortran or C pre-processed to identify inputs and outputs of interest
 - Automatic differentiation software (such as ADIFOR, OpenAD, TAMC) processes the code, adding derivatives for each elementary function.
 - As processed code runs, the derivative is obtained by chain rule
- **Forward mode: follows the flow of the program, computes direct derivative of every output with respect to a selected input.**
- **Reverse mode: records the flow of the program then reverses it, computes adjoint derivative of a selected output with respect to all inputs.**



Application of Automatic Differentiation

- **AD has been applied to a simplified model of reactor heat removal combined with the point-kinetics reactivity feedback module from SAS4A/SASSYS-1.**
- **Goal is to obtain derivatives of reactor core temperatures with respect to uncertainties in reactivity feedback coefficients during an unprotected loss of flow.**
- **Inconvenient details:**
 - 10k lines of Fortran 77 code
 - Use of equivalence statements and common blocks
 - Subroutines with variable number of parameters
 - Direct memory references, variable offset computations, memory copy operations.
- **Status: problematic language constructs rewritten, processed code compiles, different AD packages agree with each other.**
- **Verification:**
 - Basic finite-differences and complex differentiation
 - Derivative estimates do not agree with finite-differences results.



High Fidelity Coupling

- **Work package scope is to accomplish the coupling of high fidelity RANS/CFD thermal-hydraulics analysis capabilities with an existing integral safety analysis computer code.**
 - Applied initially to multidimensional simulation of reactor coolant flow in ex-core volumes (plenums).
 - Provide much better resolution of multidimensional temperature and flow fields, especially during low flow conditions that result in thermal stratification.
- **Thermal stratification (outlet plenum or cold pool).**
 - Impacts natural circulation driving forces, reactor vessel expansion, control-rod driveline expansion, IHX performance, pump inlet conditions, RVACS heat rejection, etc.
- **Current transient safety capabilities limited to perfect mixing or coarse, 1-D treatment.**
 - 1-D treatment is currently limited to three, discrete, stratified layers.
 - Correlations are used for incoming jet flow and entrainment.

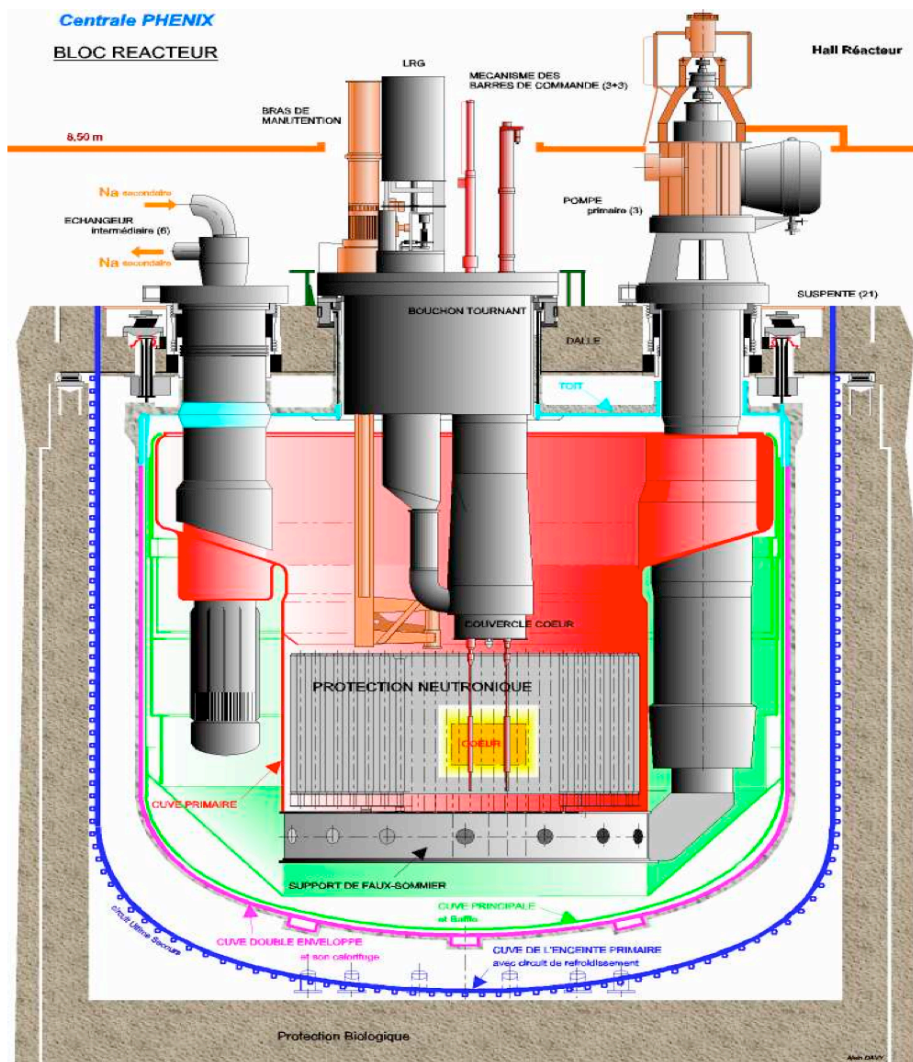


Tasks and Milestones

- **Definition of the coupling technique**
- **Implementation of coupling mechanisms**
 - Implemented with the SAS4A/SASSYS-1 and STAR-CD codes.
- **Demonstration of the coupled capability with prototypic application**
 - Identified Phenix EOL Natural Convection test for demonstration
 - *Integrates well with the International Passive Safety work package.*
 - *Opportunity to compare with experimental data.*
 - *Incomplete benchmark specifications affect ability to develop realistic models.*
 - Obtained permission from Toshiba (through CRIEPI) to use 2006 4S plenum design description.
 - *Ongoing collaboration between ANL and CRIEPI to perform comparisons between SAS4A/SASSYS-1 and CERES.*
 - *Impact of thermal stratification on natural circulation flow rates and core outlet temperatures had been identified as an issue.*
- **Milestone Reports:**
 - July 2009: Coupling of High Fidelity and Integral Analysis Methods Report
 - September 2009: Report on Prototypic Analyses Demonstrating Coupled Safety Modeling



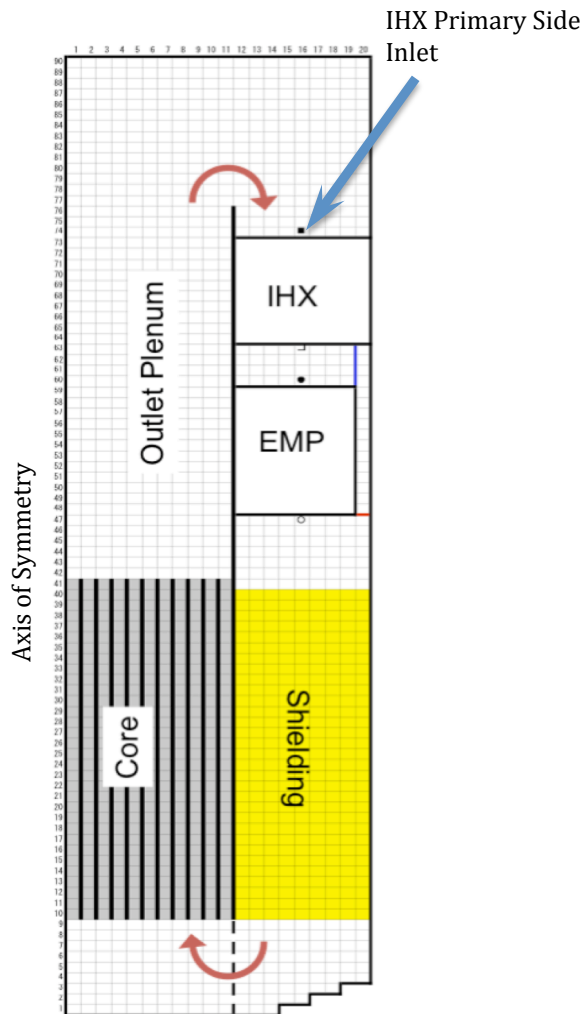
Phenix End of Life Testing



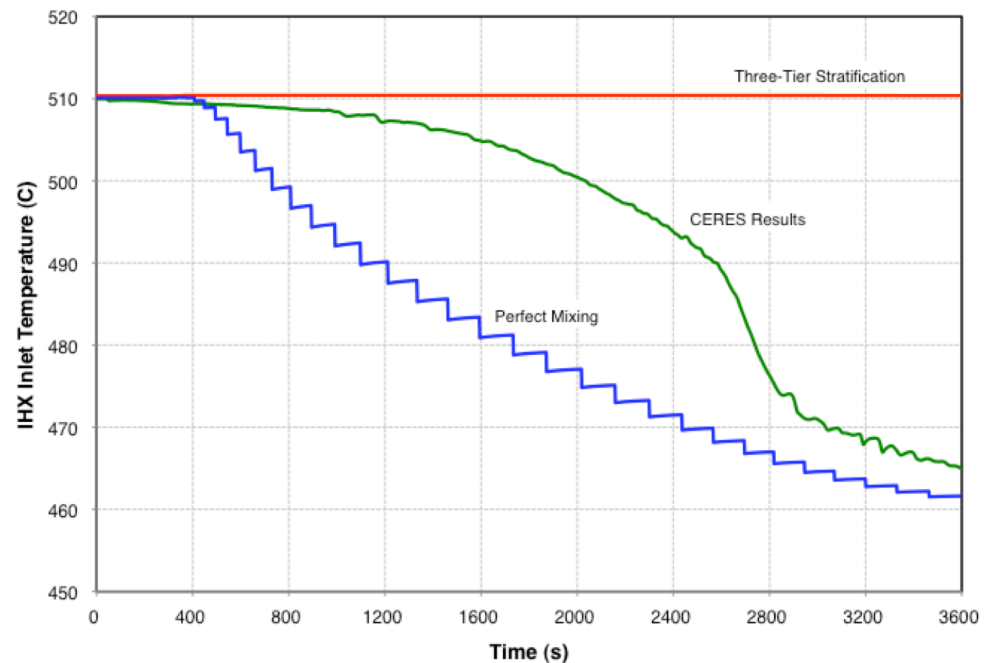
- Natural convection test will provide data on primary system natural circulation flow rates following a steam generator dryout accident with manual scram and pump trip.
- SAS4A/SASSYS-1 is being used to evaluate flow conditions as part of the IAEA CRP benchmark.
- Axial thermocouple probes will be inserted in both the hot and cold pools prior to the test.
- Provides an opportunity to compare higher-fidelity plenum modeling results with actual plant data.
 - Axial temperature distributions.
 - Impact of stratification on natural circulation development.
- Incomplete benchmark specifications affect ability to develop realistic models.



Toshiba 4S Outlet Plenum Stratification



- Previous work with CRIEPI compared system-wide results from PLOF and ULOF accident sequences.
- Plenum results from the 2-D treatment (CERES) fall between SAS4A/SASSYS-1 stratified model (blue) and a perfect mixing model (red) during a PLOF.
- More detailed treatment may reveal better mixing than CERES results predict.

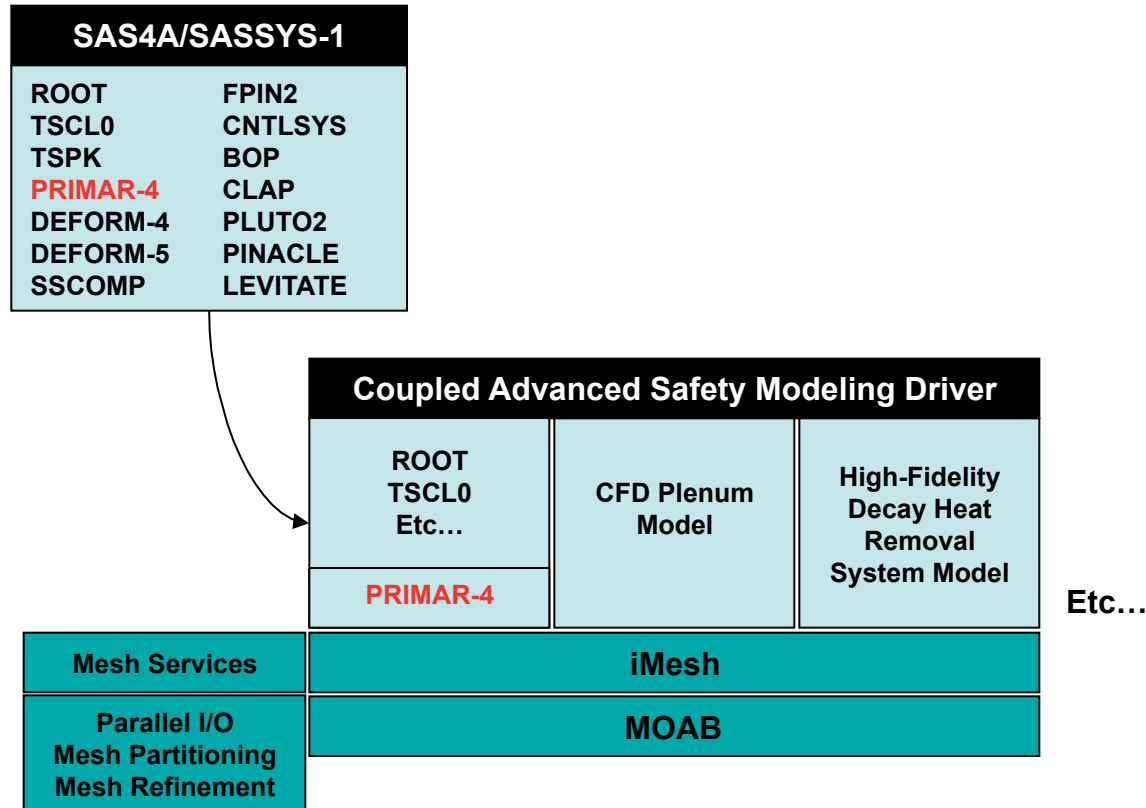


Impact of Stratification on IHX Inlet Temperatures



Safety Modeling in the SHARP Framework

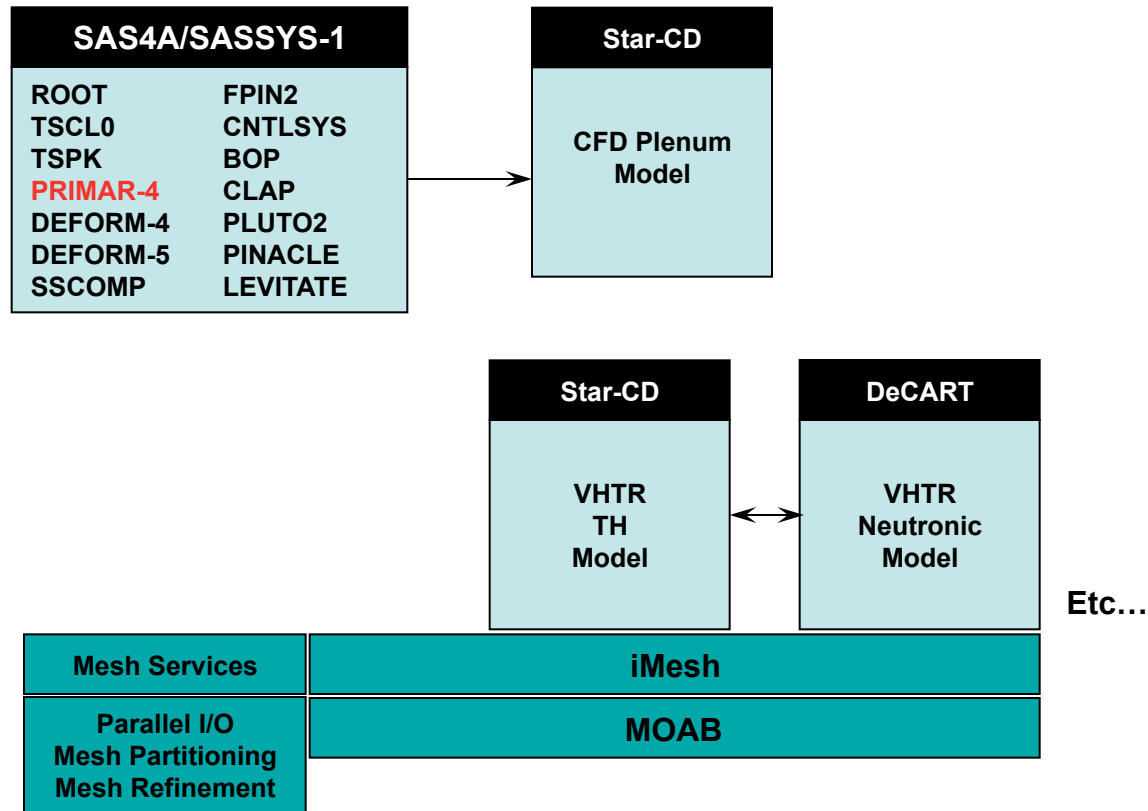
- PRIMAR-4 implements the ex-core TH modeling capabilities of SAS4A/SASSYS-1.
- Long-range goal is to couple SAS4A/SASSYS-1 into the SHARP simulation framework through PRIMAR-4 in order to provide whole-plant capabilities to support development of advanced methods.





Initial Plenum Model Coupling

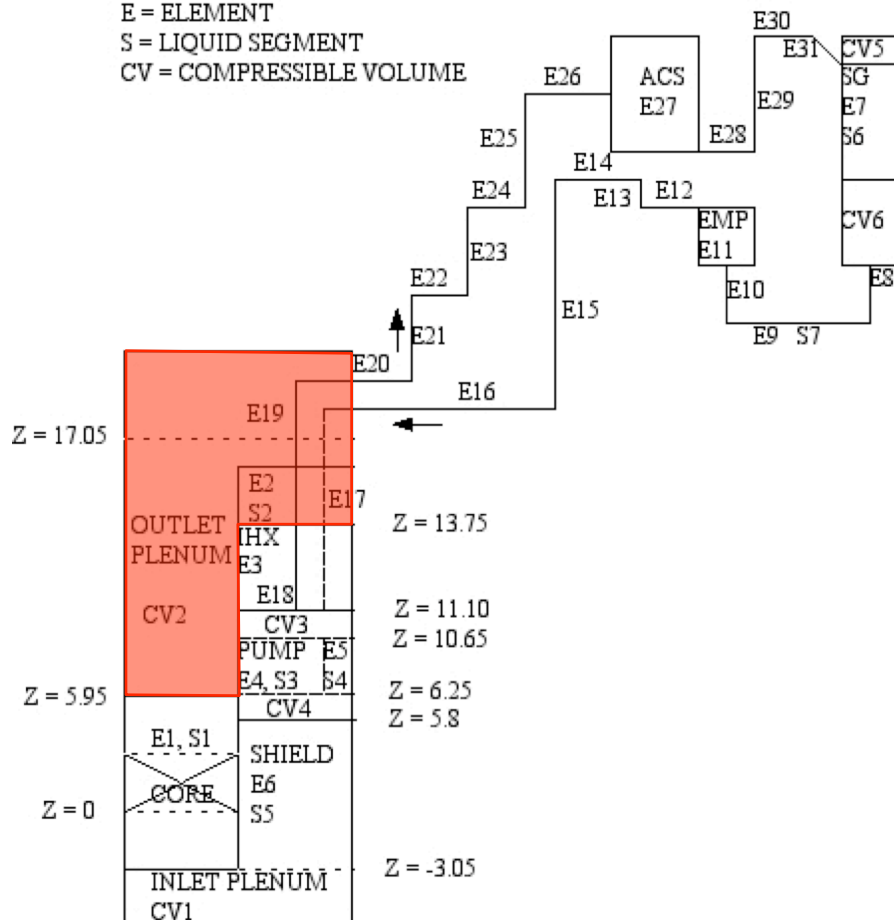
- Initial coupling between SAS4A/SASSYS-1 and Star-CD will be separate from the SHARP framework.
- Coupling will eventually leverage ongoing work to couple Star-CD with the SHARP framework under the VHTR program.





Whole-Plant Represented by SAS4A/SASSYS-1 Model

E = ELEMENT
S = LIQUID SEGMENT
CV = COMPRESSIBLE VOLUME



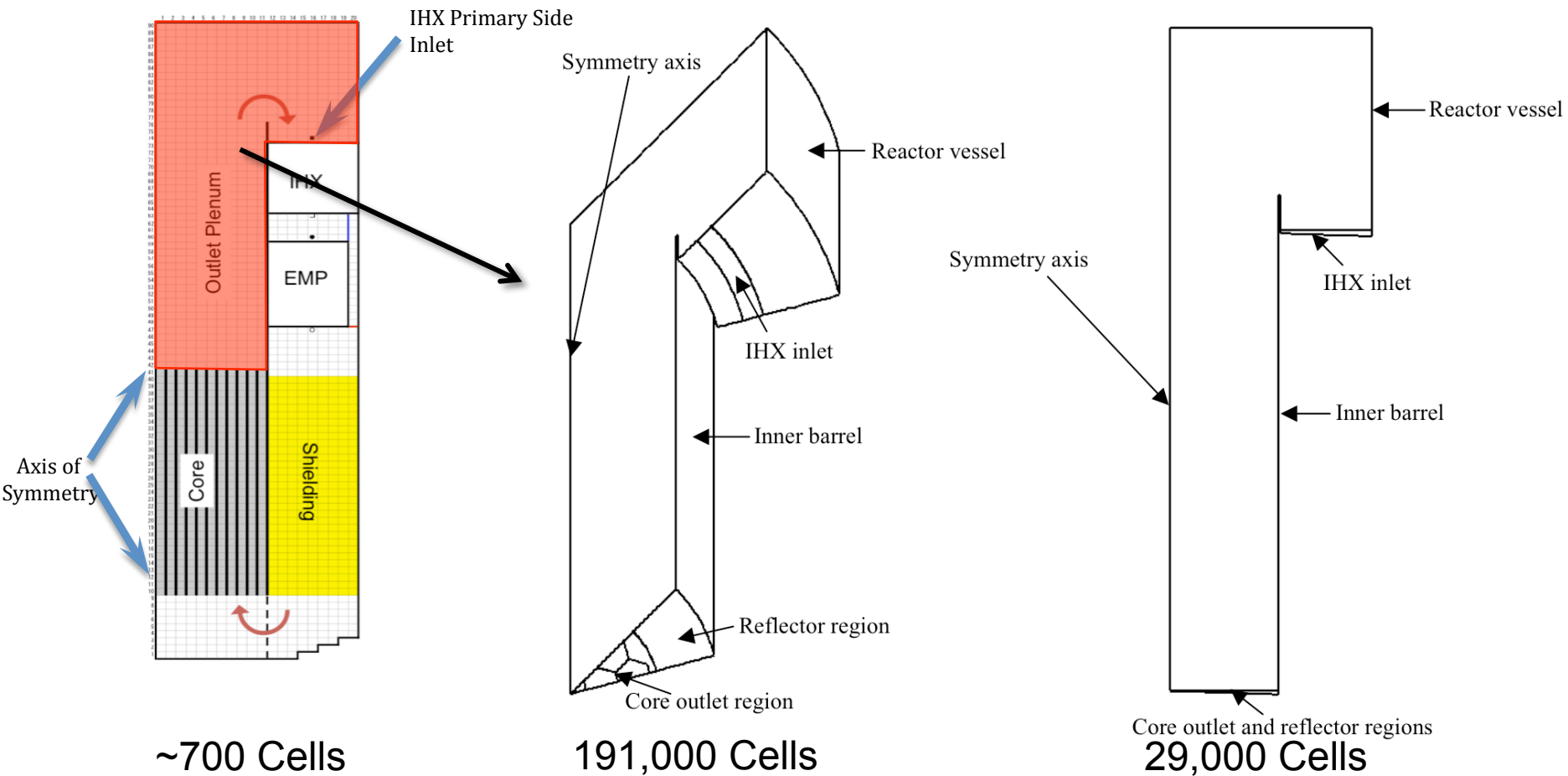
- Whole-plant discretization by CFD is beyond current computing capabilities.
- Core channel model represents central shutdown assembly; inner, middle, and outer core assemblies; and radial reflector.
- PRIMAR-4 employs a modular network of compressible volumes connected by liquid flow segments.
 - Inlet and outlet plenums.
 - IHX, EMP, SG, RVACS, IRACS, piping, shields, etc.
- Compressible Volumes:
 - Quasi one-dimensional.
 - Single temperature (perfectly mixed).
 - Single pressure at reference elevation.
 - Gravity head adjustments for inlet and outlet elevations.
 - Include dV/dT_w and dV/dP effects.



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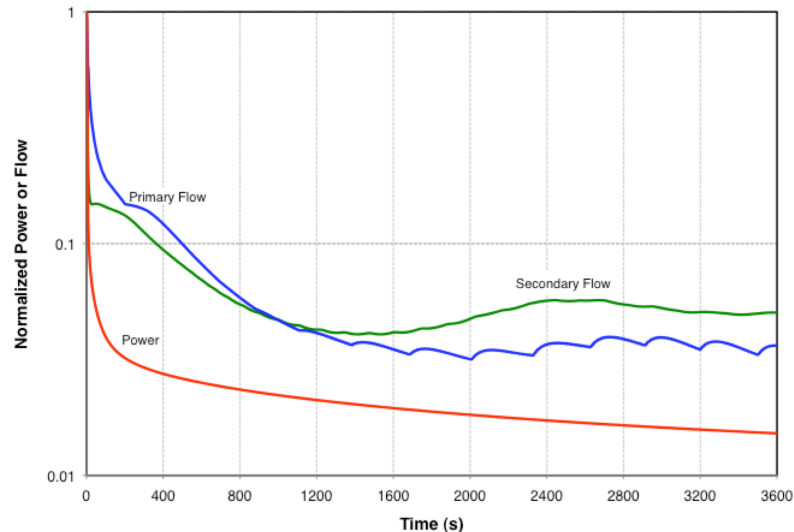
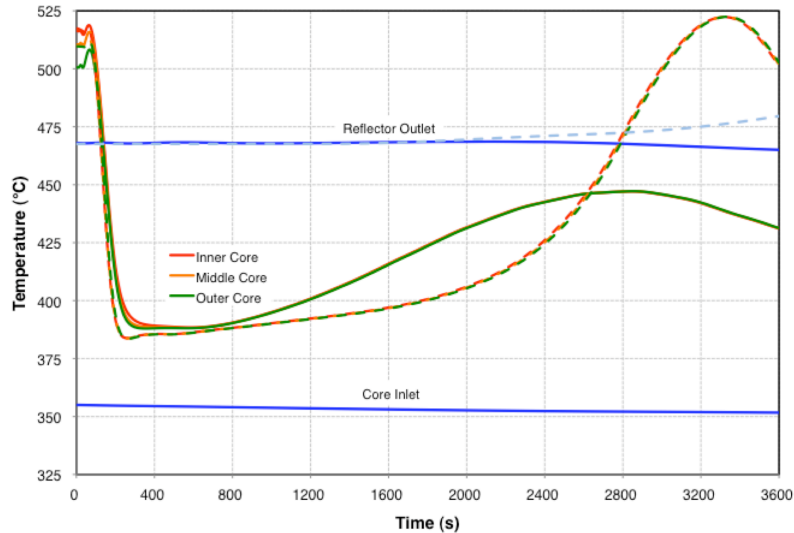
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Outlet Plenum Represented by 3-D or 2-D CFD Model





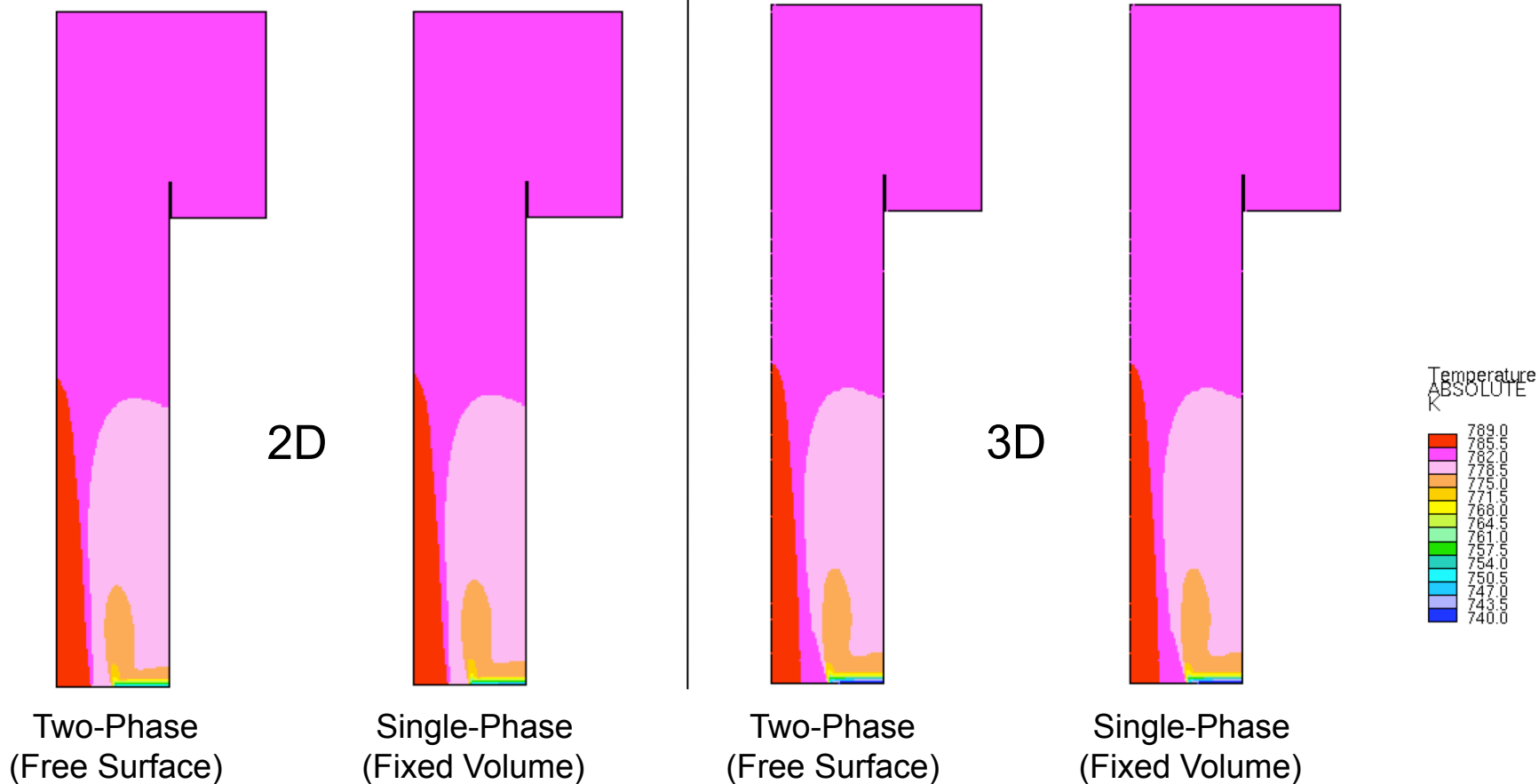
Treatment of Boundary Conditions



- Initial coupling is one way:
SAS4A/SASSYS-1 → STAR-CD
Thermal feedback is not considered.
 - Valid during steady-state (well mixed)
 - Valid during initial pump coast-down (not buoyancy driven)
 - Not valid at later times
- Effects of model assumptions and fidelity on thermal stratification, flow distributions, and primary-side IHX inlet temperatures can be evaluated independently.
- Individual core assembly flow rates and temperatures are used as boundary conditions for the STAR-CD CFD simulation.
- For the free surface simulation, outflows to the IHX provide an additional boundary condition.

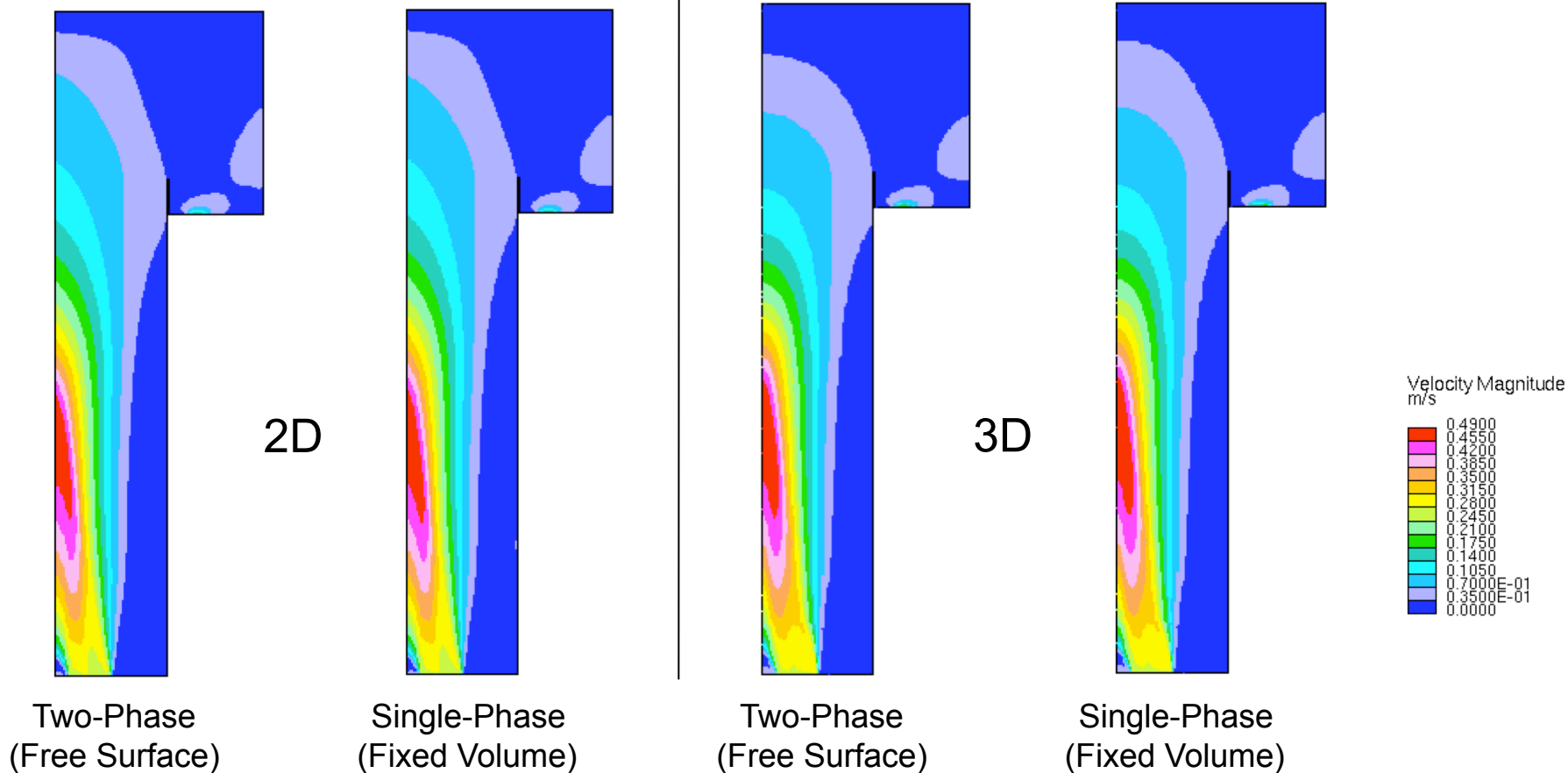


Steady State Temperature Distributions



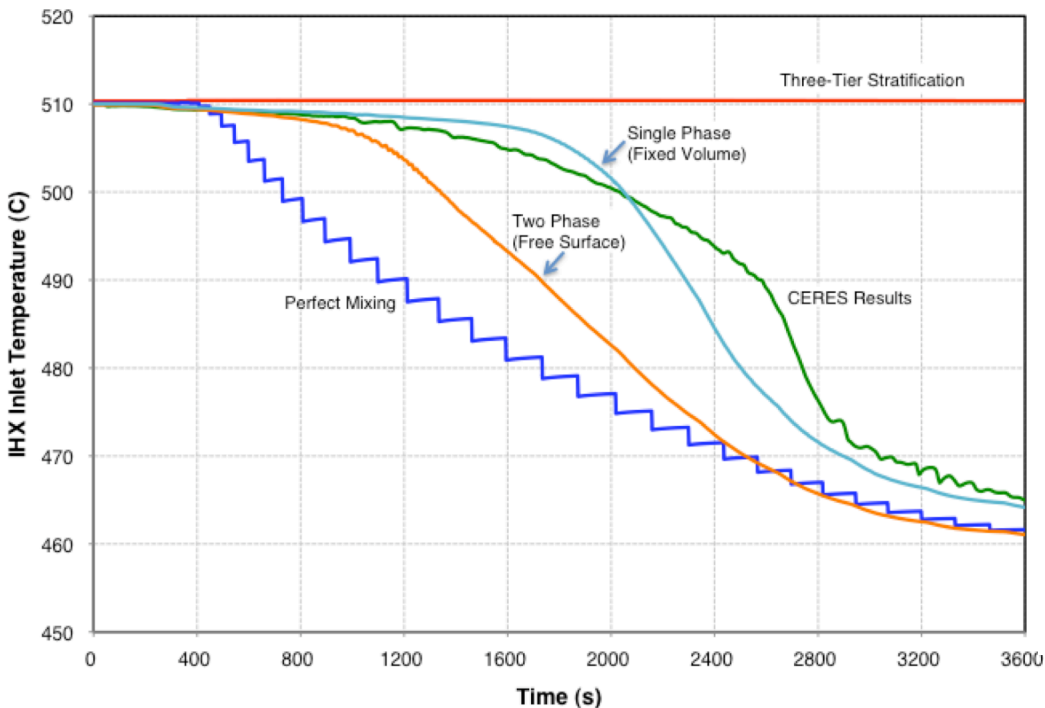


Steady State Velocity Magnitude





Transient Primary-Side IHX Inlet Temperatures

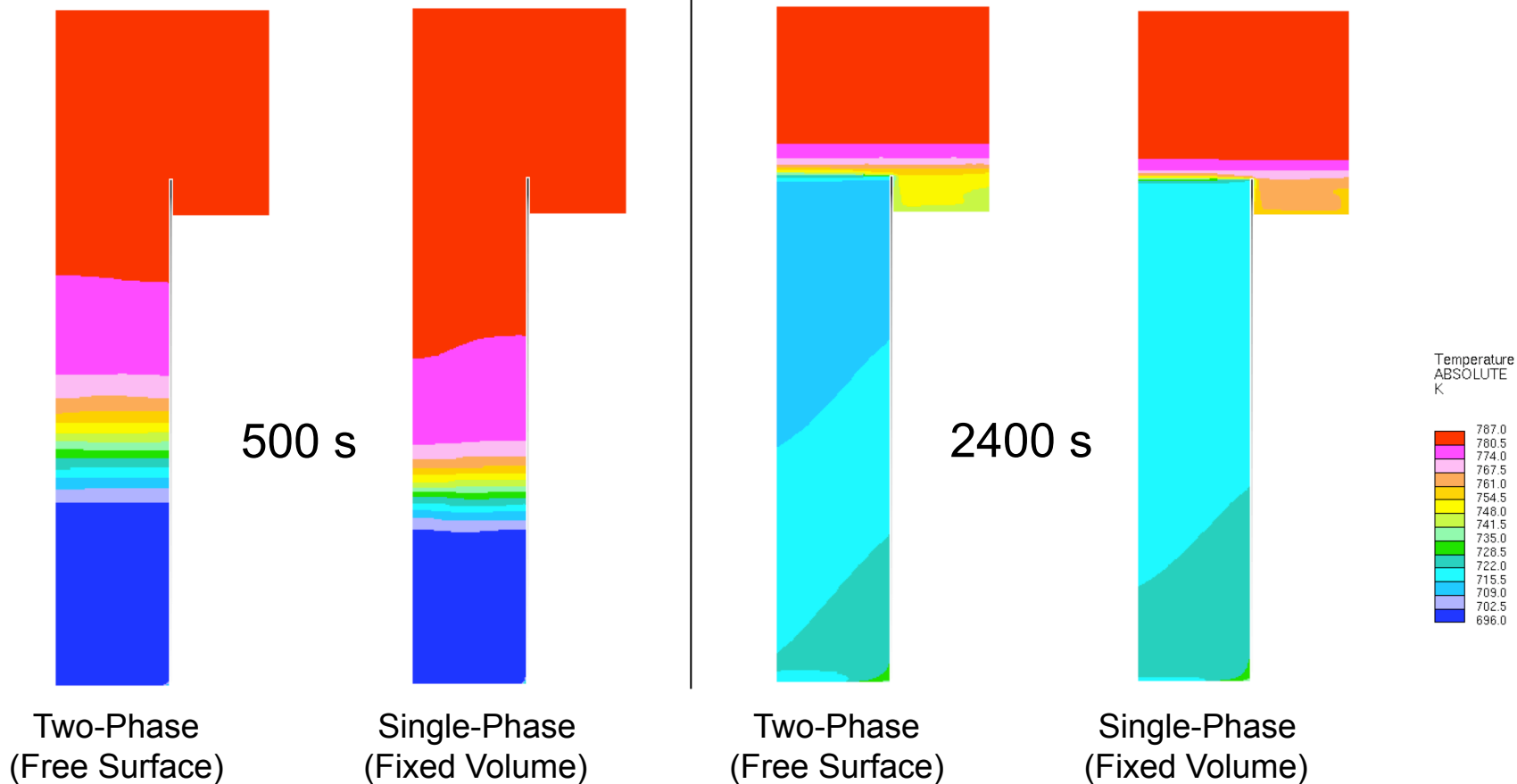


Model	Number of Processors	CPU Time (hours)	Total Time (hours)
SAS4A/SASSYS-1 (0 – 3600 s)	1	< 1 min	< 1 min
2-D Axisymmetric, VoF (cover gas)			
Stage 1 (0 – 1535 s)	8	187.4	239.3
Stage 2 (1535 – 3600 s)	12	90.3	137.4
Total		277.7	376.7
2-D Axisymmetric, Single Phase			
Stage 1 (0 – 1000 s)	12	84.3	86.2
Stage 2 (1000 – 2000 s)	12	23.8	25.3
Stage 3 (2000 – 3000 s)	12	21.0	22.4
Stage 4 (3000 – 3600 s)	12	5.3	5.4
Total		134.4	139.3

- Only the 2-D were used to compute the full transient.
- Calculation of initial flow coast down dominates computing time.
- Treatment of free-surface motion results in significant increase in thermal mixing throughout the plenum.
 - Converges to perfect mixing results by 2400 seconds.
- Single phase model is generally consistent with the results from CERES.

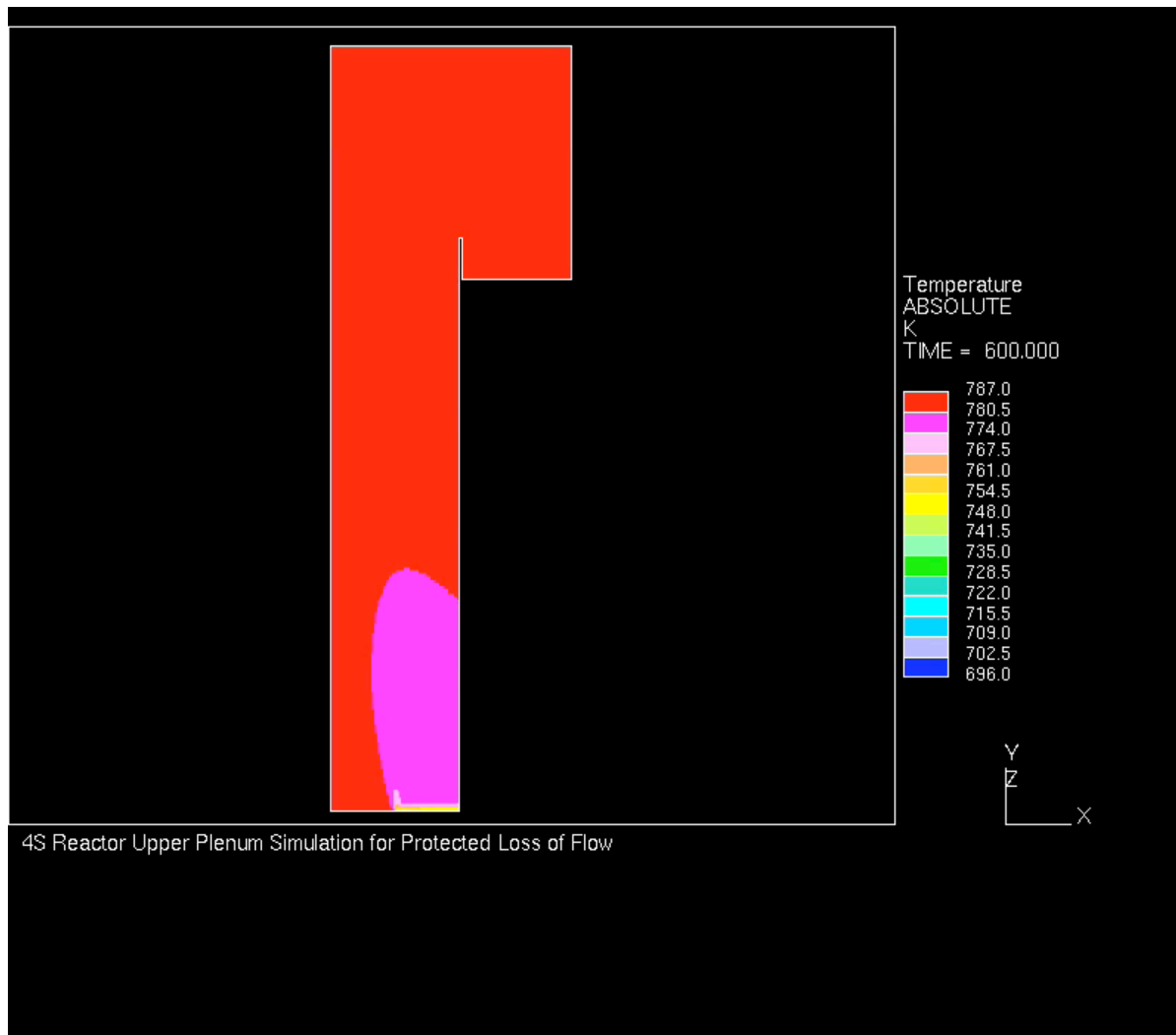


Transient Temperature Profiles





Transient Temperature Profiles





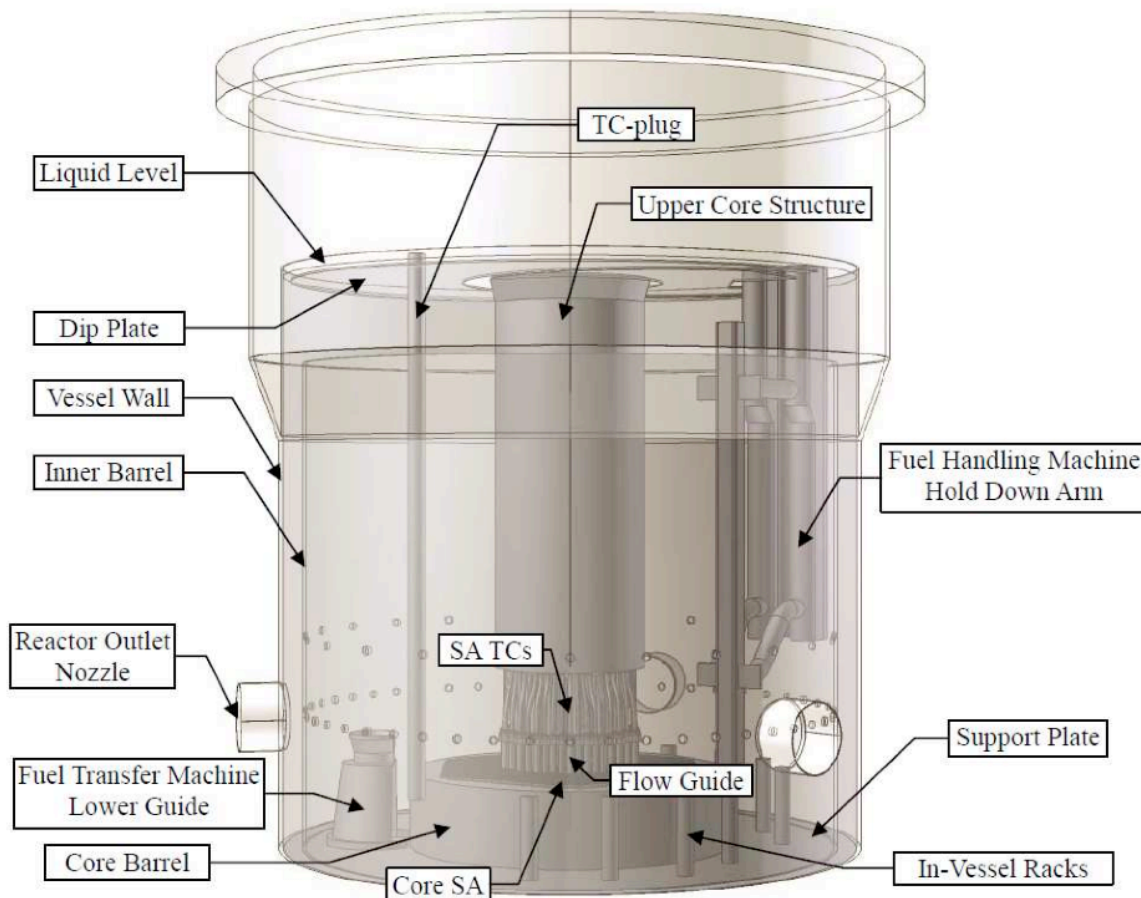
Future Directions

- **Initial scope of future work will be to include thermal feedback in the SAS4A/SASSYS-1/STAR-CD coupling.**
 - Assess the impact on natural circulation flow rates in the PLOF and ULOF transient for 4S.
 - Compare with CERES results.
- **With enhanced coupling, contribute additional results for the Phenix end-of-life natural convection test.**
 - Ongoing International Passive Safety Benchmark.
 - Next IAEA RCM in two weeks.
- **Other opportunities:**
 - Monju hot pool stratification during startup testing (also IAEA benchmark)
 - EBR-II cold pool stratification during PICT or SHRT testing (future benchmark?)



Monju Startup Testing

- Shutdown transients showed that inner barrel bypass holes influenced thermal stratification.

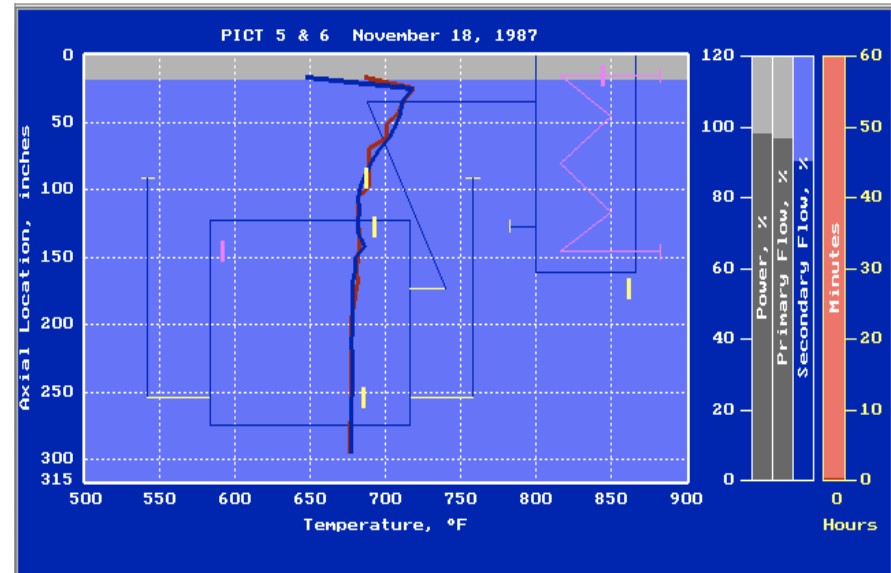


- Passive safety evaluations were performed under the Reactor Campaign as part of an IAEA benchmark, but whole-plant (or even core) model was not included.
- Additional core and primary system modeling information would be needed.
- Milestone M2505070101



EBR-II Cold Pool Stratification

- Thermocouple probes present in the EBR-II cold pool during PICT testing show thermal stratification during normal operations.
- Thermal stratification gradient begins to increase near the primary pump inlet.
- Behavior of the stratified layer during a transient may affect passive safety performance by impacting core inlet temperatures.
 - Natural circulation flow rates.
 - Core radial expansion.
- Current year milestone M3505070201 in the Reactor Campaign documents the availability of EBR-II passive safety test results.

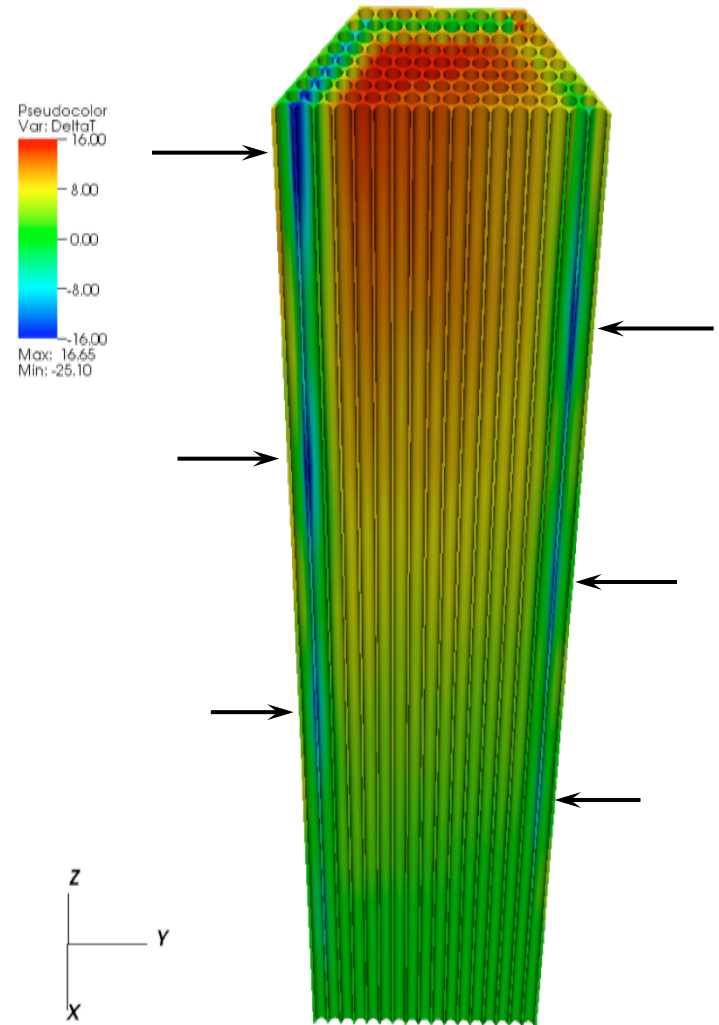


Thermocouple Probe Temperatures
During EBR-II Plant Inherent Control Tests



Future Directions (continued)

- **Evaluate methods for determining subchannel model coefficients based on LES- or RANS-averaged cross flow terms.**
 - As part of multiresolution approach, improve existing subchannel model results.
 - Also need to improve RANS results (from FY08).
- **Begin development of fast-running, modest-fidelity, whole-assembly, transient thermal-hydraulic modeling capability.**
 - Developed within the SHARP framework.
 - Support coupling with whole-plant systems code.
 - Replace existing subchannel models.
 - Ultimate goal is high-fidelity, whole-core *transient* simulation capability.



Differences Between Steady-State Subchannel and RANS Coolant Temperature Distributions in a 217-Pin Fuel Bundle.



Future Directions (continued)

- **Continue initial work on application of automatic differentiation tools to simplified systems codes.**
 - Identify coding practices needed to facilitate AD of future modeling capabilities.
- **Perform Monte-Carlo-based sensitivity analysis of a whole-plant transient by coupling GoldSim with SAS4A/SASSYS-1.**
 - Assess sensitivity of fuel/clad/coolant temperatures on subchannel cross flow or cross-pin conduction.
 - Assess sensitivity of transition to natural circulation as a function of core and IHX configuration would also be possible.



Summary

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- **Coupling between an existing, whole-plant systems code and a high-fidelity CFD code has been carried out.**
 - Evaluate the conditions of outlet plenum thermal stratification during a long-term PLOF.
 - Modeling treatment (free surface vs. single phase) has a considerable impact on thermal mixing.
- **Future coupling efforts will include thermal feedback.**
 - Assess impact on natural circulation flow rates.
 - Opportunities for additional participation in international passive safety benchmarks (Phenix, Monju, EBR-II).
- **In addition to ex-core plenum volumes, development of improved in-core *whole assembly* models is planned.**
 - Replace existing subchannel models (fuel bundle only)
 - Support high-fidelity, whole-core transient capability.
- **Sensitivity Analysis:**
 - Continue initial work on application of automatic differentiation.
 - Perform Monte-Carlo-based sensitivity analysis of a whole-plant transient